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Solvable model for three-dimensional quantum scattering of a particle off several separable interactions centred at n arbitrary points

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Abstract. A solvable model for non relativistic quantum scattering in three-dimensional space of a particle off several interactions centred at n arbitrary points is given. The interaction at one centre can be very different from the interaction at another. Each interaction centred at a given point can be effective on any partial wave with respect to this point. Each centred interaction is a sum of projectors on a finite number of partial waves relative to the centre. Elementary applications are given.

1. Introduction

A solvable model for scattering of a particle off many centres is known under various names such as 'point interactions, zero-range potentials, delta interactions, Fermi pseudopotentials, ...'. This model is analysed and reviewed in detail by Albeverio *et al* [1]. In this model, each interaction at the point P_j is $\alpha_j \delta^d(\boldsymbol{r} - \boldsymbol{a}_j)$ with $\boldsymbol{a}_j$ the vector from an origin to the point P_j, and d the dimension of the space. Each interaction is thus parametrized by a single parameter, α_j, and in three-dimensional space, ($d = 3$), each point interaction is effective only on the s partial wave ($\ell = 0$) relative to this point. For the wide field of applications in physics of these zero-range potentials, we refer to [1].

We present in this paper another solvable model, in three-dimensional space. The total interaction is the sum of n interactions centred at n arbitrary points. The interactions centred at different points can be very different from each other. The interaction centred at a given point (or centre), is of non-zero range and can involve any partial wave (relative to this centre). A detailed presentation of the total interaction is given in section 2. From a mathematical point of view, this model appears simpler than the zero-range model because each interaction is less singular. Roughly speaking, only one Dirac distribution is involved whereas three are needed by the zero-range potentials in three-dimensional space. This model is also more 'flexible' than the zero-range model in the sense that it can describe a much larger class of interactions. It is nevertheless best suited for the description of short-range interactions for low-energy processes, because in these situations the results are simpler.

By solvable model, we mean a model where the scattering amplitude can be expressed explicitly in terms of well known functions (specifically: spherical Bessel functions, spherical harmonics, $so(3)$ Clebsch–Gordan coefficients). To compute effectively the

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scattering amplitude, one has however to solve a linear system of algebraic equations. The order of this system increases linearly with the number of scattering centres.

Although the main purpose of this paper is to present the model, elementary applications are presented in section 4 for the purpose of illustration.

2. The overall interaction

$$V = \sum_{j=1}^{n} V_j. \tag{1}$$

Points of the space will be referred to with respect to an arbitrary chosen right-hand orthonormal frame of axes x, y, z with origin O. The interaction V_j is centred on the point P_j defined by the vector equation

$$\vec{OP}_j = \boldsymbol{a}_j. \tag{2}$$

A one to one correspondence between points and indices is assumed: if $j \neq s$ then also $\boldsymbol{a}_j \neq \boldsymbol{a}_s$. We use units such that $\hbar = 1, e = 1, m_{e^-} = 1$ (atomic units). The interaction V_j is defined by

$$V_j = \sum_k \lambda_j^k |\xi_j^k\rangle\langle\xi_j^k| \tag{3}$$

$$|\xi_j^k\rangle = \exp(-\mathrm{i}\boldsymbol{a}_j \cdot \boldsymbol{p})(r_j^k)^{3/2}|r_j^k, \ell_j^k, m_j^k\rangle. \tag{4}$$

The vector $|r_j^k, \ell_j^k, m_j^k\rangle$ is a generalized vector, i.e. the norm involves a distribution. Normalization and phase conventions are summarized in appendix A. The vector $|r_j^k, \ell_j^k, m_j^k\rangle$ is an eigenvector of the squared orbital angular momentum with eigenvalue $\ell_j^k(\ell_j^k + 1)$, an eigenvector of the component L_z of the orbital angular momentum with eigenvalue m_j^k, and a generalized eigenvector of the radial position operator with generalized eigenvalue r_j^k. All operators are relative to the frame O, x, y, z.

The momentum operator is denoted by $\boldsymbol{p}$. The exponential term in equation (4) corresponds to a translation by a vector displacement $\boldsymbol{a}_j$. The lower index (presently j) corresponds to the position of the centre of the interaction V_j. The variation range of the upper index (presently k) depends on the point P_j. The interaction V_j is thus the sum of separable interactions centred on the point P_j, of range r_j^k, of strength λ_j^k.

The question now may arise, of how a given central potential W of range r_0 can be approximated by our nonlocal interactions. From the equation (see appendix A):

$$W = \int_0^{r_0} \mathrm{d}r\, r^2 \sum_{\ell,m} W(r)|r, \ell, m\rangle\langle r, \ell, m|$$

it is seen that W can effectively be approximated by a finite sum of separable interactions if the integral is approximated by a discrete sum and if the infinite summation over the partial waves is replaced by a finite summation up to a maximum value $\ell_{\max}$. The value of $\ell_{\max}$ will increase with the energy of the collision, and at very low energy, one has $\ell_{\max} = 0$.

3. Solution of the scattering problem

Let M denote the mass of the particle and $p_0^2/(2M)$ its kinetic energy when it moves freely, long before or after the collision. It is well known (see e.g. [2]) that the complete solution of the scattering problem is determined if the operator

$$T(z) = V + VG(z)V \tag{5}$$

is known. The operator $G(z)$, called the resolvent or Green operator, is defined by

$$G(z) = [z - p^2/(2M) - V]^{-1}. \tag{6}$$

The existence of $G(z)$ and therefore of $T(z)$ requires of course that z does not belong to the spectrum of the total Hamiltonian $p^2/(2M) + V$. The scattering amplitude $f(\boldsymbol{p}' \leftarrow \boldsymbol{p})$, corresponding to initial momentum $\boldsymbol{p}$, and final momentum $\boldsymbol{p}'$ with $\boldsymbol{p} \cdot \boldsymbol{p} = \boldsymbol{p}' \cdot \boldsymbol{p}' = p_0^2$, is given by:

$$f(\boldsymbol{p}' \leftarrow \boldsymbol{p}) = -(2\pi)^2 M \lim_{\epsilon \to 0^+} \langle \boldsymbol{p}' | T(p_0^2/(2M) + \mathrm{i}\epsilon) | \boldsymbol{p} \rangle$$

where $\lim_{\epsilon \to 0^+}$ means that ϵ goes to zero and is positive. The scattering amplitude $f(\boldsymbol{p}' \leftarrow \boldsymbol{p})$ contains all the information. In particular, the differential cross section can be expressed as

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\boldsymbol{p}' \leftarrow \boldsymbol{p})|^2.$$

Integration over the solid angle Ω yields the integrated (or total) cross section which can also be obtained more easily from the optical theorem

$$\sigma = \frac{4\pi}{p_0} \Im(f(\boldsymbol{p} \leftarrow \boldsymbol{p})). \tag{7}$$

The algebraic identity

$$G(z) = G_0(z) + G_0(z) V G(z) \tag{8}$$

with

$$G_0(z) = [z - p^2/(2M)]^{-1} \tag{9}$$

leads generally to an integral equation for the matrix elements of $G(z)$. This equation, called the Lippman–Schwinger equation, is generally very difficult to solve. For the interaction (1) which according to equation (3) is the sum of separable interactions, only the matrix elements $\langle \xi_j^k | G(z) | \xi_q^r \rangle$ are required for the determination of $T(z)$ (see equation (5)). Moreover, the determination of these matrix elements by using equation (8) reduces to solving a linear system of algebraic equations if the matrix elements $\langle \xi_j^k | G_0(z) | \xi_q^r \rangle$ are known. Specifically, if all $|\xi_q^r\rangle$ are indexed by a different integer ($|J\rangle \equiv |\xi_q^r\rangle$) running from unity up to the total number N of different $|\xi_q^r\rangle$, one has to solve the matrix equation: $g = b^{-1} g_0$ with the N order matrices defined by $g_{IJ} = \langle I | G(z) | J \rangle$, $(g_0)_{IJ} = \langle I | G_0(z) | J \rangle$, $b_{IJ} = \delta_{IJ} - \lambda_J \langle I | G_0(z) | J \rangle$ where δ_{IJ} is the Kronecker symbol. For the interaction given by equations (1), (3) and (4) it is shown in appendix B that the matrix elements $\langle \xi_j^k | G_0(z) | \xi_q^r \rangle$ can be determined analytically (see equations (42) and (45)). Equation (45) is the key result that allows a complete analytical solution of the model. This equation has been derived under the conditions (44) which express the fact that interactions centred on different points must not overlap. The case of overlapping interactions yields a different result which could also be computed analytically.

4. Applications

From now on, we define $\sqrt{z}$ as the square root with a positive imaginary part, and, when z is a real positive number, as $\lim_{\epsilon \to 0^+} \sqrt{z + \mathrm{i}\epsilon}$. The relation between z and momentum p is given by

$$p \equiv \sqrt{2Mz}. \tag{10}$$

Thus, for notational convenience, p is used in place of p_0 and it should be clear from the context when p denotes an operator or a number.

For applications we shall limit ourself to the cases where each centred interaction V_j is invariant by time reversal and rotation about its centre. The centred interactions V_j (equation (3)) are not necessarily invariant by time reversal, nor by rotation. The constraints on V_j in order to satisfy these symmetries are discussed in appendix C.

4.1. Scattering off a single centre

It is important first to study thoroughly the scattering off a single centre in order to appreciate the signification of each centred interaction. For a single centre, there is only one term V_1 in equation (1). For the sake of simplicity we shall only consider the case where there is only one range, r^ℓ, for each partial wave ℓ. The origin of space is arbitrary and we choose therefore $\boldsymbol{a}_1 = 0$.

$$V = V_1 = \sum_\ell \lambda^\ell (r^\ell)^3 \sum_{m=-\ell}^{\ell} |r^\ell, \ell, m\rangle\langle r^\ell, \ell, m|.$$

The symbol ℓ in $(r^\ell)^3$ is an upper index, the number 3 an exponent. The interaction V is thus the sum of projectors on different partial waves, and the scattering amplitude is decomposed as:

$$f(\boldsymbol{p}' \leftarrow \boldsymbol{p}) = \sum_\ell (2\ell+1) f_\ell(p) P_\ell(\cos(\theta))$$

with $0 \leqslant \theta \leqslant \pi$ the angle between initial and final momenta $\boldsymbol{p}, \boldsymbol{p}'$. The equations (5), (6), (8) and (9) yield

$$T(z) = \sum_\ell \sum_{m=-\ell}^{\ell} \frac{(r^\ell)^3 |r^\ell, \ell, m\rangle\langle r^\ell, \ell, m|}{\frac{1}{\lambda^\ell} - (r^\ell)^3 \langle r^\ell, \ell, m|G_0(z)|r^\ell, \ell, m\rangle} \tag{11}$$

and, using the addition theorem for spherical harmonics, and equation (42), the partial-wave scattering amplitude is given by

$$f_\ell(p) = -\frac{j_\ell^2(pr^\ell)}{\frac{1}{2M(r^\ell)^3\lambda^\ell} + p j_\ell(pr^\ell) h_\ell^+(pr^\ell)}. \tag{12}$$

For the sake of completeness we also give the explicit expression of the stationary scattering partial-wave states defined by

$$|p, \ell, m, +\rangle = |p, \ell, m\rangle + G_0(z)T(z)|p, \ell, m\rangle.$$

One obtains

$$\langle r, \ell, m|p, \ell, m, +\rangle = \mathrm{i}^\ell \sqrt{\frac{2}{\pi}} \left\{ j_\ell(pr) - \frac{j_\ell(pr^\ell)}{\frac{1}{\lambda^\ell 2M(r^\ell)^3} + p h_\ell^+(pr^\ell) j_\ell(pr^\ell)} p h_\ell^+(pr_\rangle) j_\ell(pr_\langle) \right\} \tag{13}$$

with $r_\langle, r_\rangle$ respectively the smallest and greatest of the two values r, r^ℓ.

It is clear from equation (11) that the poles of the T-operator, or equivalently the poles of the resolvent are given by the equation

$$1/\lambda^\ell = (r^\ell)^3 \langle r^\ell, \ell, m|G_0(z)|r^\ell, \ell, m\rangle. \tag{14}$$

It can be shown (see e.g. [3]) that a separable interaction $\lambda|\xi\rangle\langle\xi|$ supports at most one bound state, and supports it when $0 \rangle 1/\lambda \rangle \langle\xi|G_0(0)|\xi\rangle$. The energy E_b of the bound state is given

by $1/\lambda = \langle\xi|G_0(E_b)|\xi\rangle$. In these cases, each partial wave interaction can support a bound state if

$$0\rangle 1/\lambda\rangle \lim_{p\to 0} -2M(r^\ell)^3 p h_\ell^+(pr^\ell) j_\ell(pr^\ell) = -2M\frac{(r^\ell)^2}{2\ell+1} \equiv \frac{1}{\lambda_c^\ell}.$$

Thus a bound state can be supported if λ^ℓ is smaller than the (negative) critical value λ_c^ℓ.

A pole of the resolvent near the real axis gives rise to a resonance in the diffusion, whose width is related to its imaginary part (in the variable $p^2/(2M)$). These poles are zeros of the denominator of equation (12), or zeros of the Jost function $\Upsilon_\ell(p)$ [2]. The explicit expression for the Jost function can be obtained from the stationary scattering partial wavefunction (13) and is, according to the general definition, given in [2]:

$$\begin{aligned}\Upsilon_\ell(p) &= 1 + \lambda^\ell 2M(r^\ell)^3 p h_\ell^+(pr^\ell) j_\ell(pr^\ell) \\ &= 1 - \frac{\lambda^\ell}{\lambda_c^\ell}\left\{\left[1 + \frac{2}{(2\ell-1)(2\ell+3)}(pr^\ell)^2 + \cdots\right]\right. \\ &\quad \left. + \mathrm{i}\frac{(pr^\ell)^{2\ell+1}}{(2\ell+1)!!(2\ell-1)!!}\left[1 - \frac{(pr^\ell)^2}{2\ell+3} + \cdots\right]\right\}. \end{aligned} \tag{15}$$

The zeros of the Jost function in the complex p-plane can be expanded as a series in the variable $y \equiv \frac{\lambda_c^\ell - \lambda^\ell}{\lambda^\ell}$ from equation (15) by taking the left-hand side equal to zero and reversing the series. One obtains a power series for $\ell = 0$:

$$p = \frac{\mathrm{i}}{r^0}\left\{-y + \frac{2}{3}y^2 - \frac{5}{9}y^3 + \frac{68}{135}y^4 - \frac{193}{405}y^5 + \mathrm{O}(y^6)\right\}$$

and a fractional power series for $\ell\rangle 0$:

$$\begin{aligned} p = \frac{1}{r^\ell}\left\{\left[\sqrt{\frac{(2\ell+3)(2\ell-1)}{2}}\,y^{1/2} + \mathrm{O}(y^{3/2})\right]\right. \\ \left. -\mathrm{i}\left[\frac{(2\ell+3)^{\ell+1}(2\ell-1)^\ell}{4(2\ell+1)!!(2\ell-3)!!2^\ell}y^\ell + \mathrm{O}(y^{\ell+1})\right]\right\}. \end{aligned} \tag{16}$$

For $\ell = 0$, the zero is on the positive imaginary axis for $\lambda^0\langle\lambda_c^0$ (i.e. $y\langle 0$), crosses the origin for $\lambda^0 = \lambda_c^0$ (i.e. $y = 0$) and moves to the negative imaginary axis for $\lambda^0\rangle\lambda_c^0$ (i.e. $y\rangle 0$). This behaviour leads to a zero energy resonance. A pole close to the origin on the negative imaginary axis of the p-plane corresponds to a pole on the real axis of the second Riemann sheet of the complex-energy plane where it is sometimes referred to as giving rise to a virtual state (see e.g. [2]). For $\ell\rangle 0$, the zeros are double. For $\lambda^\ell\langle\lambda_c^\ell$ one is on the positive imaginary axis, the other on the negative imaginary axis. They move toward the origin when λ^ℓ increases and cross the origin for $\lambda^\ell = \lambda_c^\ell$. Then, for $\lambda^\ell\rangle\lambda_c^\ell$, they move tangentially to the real axis with a negative imaginary part, giving rise to a nonzero energy resonance. As the imaginary part varies as y^ℓ, the widths of the resonances decrease rapidly as ℓ increases.

This different behaviour is not specific to the present model interaction but is a general property (see e.g. [2]). The series for the zero of the Jost function can, however, be computed to arbitrary precision for arbitrary fixed ℓ-value for the present model. For example, for $\ell = 1$

$$\begin{aligned} p = \frac{1}{r^1}\left\{\left[\frac{\sqrt{5}}{\sqrt{2}}\left(y^{1/2} - \frac{2215}{4032}y^{3/2} + \frac{104\,725}{221\,184}y^{5/2} - \frac{217\,723\,897\,375}{480\,687\,685\,632}y^{7/2} + \cdots\right)\right]\right. \\ \left. +\mathrm{i}\left[-\frac{25}{24}y + \frac{4775}{6048}y^2 - \frac{4431\,775}{6096\,384}y^3 + \frac{572\,969\,875}{804\,722\,688}y^4 + \cdots\right]\right\}. \end{aligned}$$

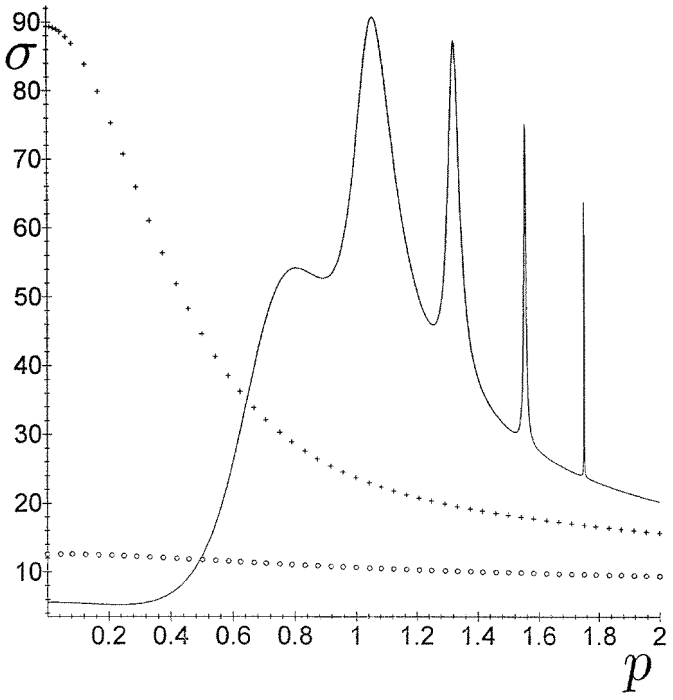

Figure 1. Total cross section σ for scattering by one centre. The abscissa corresponds to the momentum p of the incident particle. The full curve represents the cross section for the interaction V_- given by equation (17). The curve with cross symbols represents the cross section for the interaction $V+$ also given by equation (17). The lower curve with circle symbols represents the cross section for the interaction V_∞ which is defined by replacing $\lambda^\ell = -(\ell + 1/2 \mp 0.3)$ in equation (17) by the limit $\lambda^\ell \to \pm\infty$.

Figure 1 reports the total cross section for a particle of mass unity for the two cases:

$$V_\mp = \sum_{\ell=0}^{5} -(\ell + \tfrac{1}{2} \mp 0.3) \sum_{m=-\ell}^{\ell} |r = 1, \ell, m\rangle\langle r = 1, \ell, m|. \tag{17}$$

The λ^ℓ values $-(\ell + 0.2)$ are then slightly above the critical values $\lambda_c^\ell = -\ell - \frac{1}{2}$ for the existence of a bound state. The five maxima in the full curve of figure 1 are resonances associated with $\ell = 1, 2, 3, 4, 5$. The width of resonances decreases as ℓ increases as is expected from equation (16). A zero-energy resonance is not manifested because $\lambda^0 = -0.2$ is far enough from the critical value $\lambda_c^0 = -\frac{1}{2}$. The curve with cross symbols in figure 1 represents the total cross section for the case $\lambda^\ell = -(\ell + 0.8)$, which are values slightly below the critical values λ_c^ℓ . It is seen that for this case, it is the $\ell = 0$ bound state and only this state near zero energy that manifests itself as a resonance in the cross section. Finally the lower curve with circle symbols represents the cross section for the case $\lambda^\ell \to \pm\infty$.

In the limit $\lambda \to -\infty$, it can be shown from the asymptotic expansions (38) and (39), and the equation (42) that the energy of the bound state $E_b = -k^2/(2M)$ verifies the equation $\lim_{\lambda\to-\infty} k/\lambda = -Mr_\ell$ for every ℓ value.

In the limit of zero-energy scattering, the s partial wave becomes predominant and we shall now consider in more detail the scattering by a single s-wave interaction. For notational convenience we omit the upper index 0 in λ^0, r^0, and add a left lower index 1

to the scattering amplitude to recall that only one centre is present:

$$ {}_1f(\boldsymbol{p}' \leftarrow \boldsymbol{p}) =_1 f_0(p) = -\frac{\left(\frac{\sin(pr)}{pr}\right)^2}{\frac{1}{2Mr^3\lambda} + p\left(\frac{\sin(pr)}{pr}\right)\left(\frac{\exp(\mathrm{i}pr)}{pr}\right)}. \tag{18} $$

In particular

$$ \lim_{p\to 0} {}_1f(\boldsymbol{p}' \leftarrow \boldsymbol{p}) = -\frac{1}{\frac{1}{2Mr^3\lambda} + \frac{1}{r}}. $$

Let us denote for future convenience by ${}_1\sigma^0(p, r, \lambda)$ the integrated (or total) cross section for s-wave scattering.

$$ {}_1\sigma^0(p, r, \lambda) = 4\pi |f_0(p)|^2 \tag{19} $$

$$ \lim_{\lambda\to\pm\infty} {}_1\sigma^0(p, r, \lambda) = 4\pi \left(\frac{\sin(pr)}{p}\right)^2. \tag{20} $$

It is seen from equation (20) that in the limit where both $\lambda \to \pm\infty$, $p \to 0$ the cross section is $4\pi r^2$, the same result as for the scattering by an impenetrable sphere of radius r (see e.g. [4]). Care should be taken with respect to the order relative to which different limits are taken. For example, the limit $p \to \infty$ in equation (20) yields a result different from the one obtained by the more physical procedure which is to first take the limit $p \to \infty$ in equations (19) and (18) and then the limit $\lambda \to \pm\infty$.

4.2. Scattering off two projectors

The interaction is defined by

$$ \begin{aligned} V &= V_1 + V_2 \\ &= \lambda_1 |\xi_1\rangle\langle\xi_1| + \lambda_2 |\xi_2\rangle\langle\xi_2|. \end{aligned} \tag{21} $$

The T operator (see equation (5)) associated with any interaction of the form given by equation (21) can be cast, after some algebraic calculation, into the form

$$ T(z) = c(z)\{T_1(z) + T_2(z) + T_1(z)G_0(z)T_2(z) + T_2(z)G_0(z)T_1(z)\} \tag{22} $$

with $T_j(z)$ the T operator corresponding to the situation where only the interaction V_j is present:

$$ T_j(z) = \frac{\lambda_j |\xi_j\rangle\langle\xi_j|}{1 - \lambda_j\langle\xi_j|G_0(z)|\xi_j\rangle} $$

and the numerical function $c(z)$ given by

$$ c(z) = \left[1 - \frac{\lambda_1\lambda_2\langle\xi_1|G_0(z)|\xi_2\rangle\langle\xi_2|G_0(z)|\xi_1\rangle}{(1 - \lambda_1\langle\xi_1|G_0(z)|\xi_1\rangle)(1 - \lambda_2\langle\xi_2|G_0(z)|\xi_2\rangle)}\right]^{-1}. $$

It is also easy to show by inspection that the expansion of $c(z)$ according to the geometric series $1/(1-x) = 1 + x + x^2 + \cdots$ in equation (22) yields

$$ \begin{aligned} T(z) = {} & T_1(z) + T_2(z) + T_1(z)G_0(z)T_2(z) + T_2(z)G_0(z)T_1(z) \\ & + T_1(z)G_0(z)T_2(z)G_0(z)T_1(z) + T_2(z)G_0(z)T_1(z)G_0(z)T_2(z) + \cdots. \end{aligned} \tag{23} $$

This is a particular case of the so-called Faddeev–Watson multiple scattering expansion (see e.g. [5]). One thus obtains the following result: *the Faddeev–Watson expansion (FWE)* (23) *converges if*

$$\left|\frac{\lambda_1\lambda_2\langle\xi_1|G_0(z)|\xi_2\rangle\langle\xi_2|G_0(z)|\xi_1\rangle}{(1-\lambda_1\langle\xi_1|G_0(z)|\xi_1\rangle)(1-\lambda_2\langle\xi_2|G_0(z)|\xi_2\rangle)}\right| < 1 \tag{24}$$

and diverges otherwise. The physical conditions corresponding to convergence or divergence will now be discussed in a particular example.

4.2.1. Scattering off two identical s-wave projectors centred on different points. The interaction is thus:

$$V = \lambda r^3\{|r,0,0\rangle\langle r,0,0| + \exp(-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p})|r,0,0\rangle\langle r,0,0|\exp(\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{p})\}.$$

Condition (24) yields in this case (see equations (43) and (46)):

$$\left|\frac{\left(\frac{\sin(pr)}{pr}\right)^2\frac{1}{p|\boldsymbol{a}_j-\boldsymbol{a}_s|}}{\frac{1}{2Mr^3p\lambda}+\frac{\exp(\mathrm{i}pr)}{pr}\left(\frac{\sin(pr)}{pr}\right)}\right|^2 \langle 1.$$

The FWE thus converges if $|\lambda|$ is sufficiently small. This was expected since when $\lambda \to 0$, the FWE becomes similar to the Born series. Whatever the value of λ, the FWE converges provided the distance between the two points is sufficiently large. It is of interest to note that the 'rapidity' of convergence is governed by the square of the inverse of the distance between the two centres. The FWE also converges if p is sufficiently large.

The general explicit result for the total cross section is rather cumbersome, and we shall only consider some limiting cases. The sum of the two interaction is of course not invariant by arbitrary rotation and not a projector on any partial wave. Let ω denotes the angle between the initial momentum $\boldsymbol{p}$ and the axis determined by the two scattering centres. The integrated cross section is denoted ${}_2\sigma^0(p,r,\lambda,a,\omega)$ with the upper 0 index to recall that each of the two interactions is a projector on the s-wave with respect to its own centre and the left index 2 to recall that two centres are present.

The general method described in section 3 and the use of the optical theorem (7) leads after tedious but elementary calculation to

$$\begin{aligned}{}_2\sigma^0(p,r,\infty,a,\omega) \equiv \lim_{\lambda\to\pm\infty}{}_2\sigma^0(p,r,\lambda,a) &= 8\pi a^2\sin^2(pr)\\ &\times[\{(pa)^2 + pa\cos(pa\cos\omega)\sin(p(a-2r)) - \sin(pr)\sin(p(2a-r))\\ &+\cos(pa\cos\omega)\sin^2(pr)\sin(pa)/(pa)\}][((pa)^2-\sin^2(pr))^2\\ &+(2pa\sin(pr)\sin(p(a-r)))^2]^{-1}.\end{aligned}$$

This cross section varies the most rapidly with energy for an initial momentum collinear with the axis ($\omega = 0$) due to the term $\cos(pa\cos\omega)$. This is a property that is not specific to the case $\lambda \to \pm\infty$. Other relations pertaining to different limits are:

$$\lim_{a\to\infty \text{ and } pa\to\infty}{}_2\sigma^0(p,r,\infty,a,\omega) = 2_1\sigma^0(p,r,\infty) \tag{25}$$

$$\begin{aligned}\lim_{pa\to 0}{}_2\sigma^0(p,r,\lambda,a,\omega) &= 4\frac{4\pi}{\left(\frac{1}{2Mr^3\lambda}+\frac{1}{r}+\frac{1}{a}\right)^2}\\ &= 4\frac{4\pi}{\left(-\frac{1}{{}_1f}+\frac{1}{a}\right)^2}\end{aligned} \tag{26}$$

$$\lim_{pa\to 0 \text{ and } a\to\infty} {}_2\sigma^0(p,r,\lambda,a,\omega) = 4_1\sigma^0(p,r,\lambda). \tag{27}$$

Equations (25)–(27) are particularly interesting since they do not involve directly the parameters of the interactions, but relate scattering data of two-centre processes to scattering data relevant to one-centre processes.

Let us now consider the poles of the resolvent, which are also the poles of the T-operator. One obtains after some calculation that the poles of these operators are determined by the two (independent) equations:

$$\frac{1}{\lambda} = -2Mr\sin(pr)\frac{pa\exp(\mathrm{i}pr) \mp \sin(pr)\exp(\mathrm{i}pa)}{p^2 a} \tag{28}$$

which have respectively the following series expansions:

$$\frac{1}{\lambda} = -2Mr^2\left(1-\frac{r}{a}\right) - \frac{Mr^3(3a^2+2r^2-4ra)}{3a}p^2 - \frac{\mathrm{i}a^2Mr^3p^3}{3} + \mathrm{O}(p^4) \tag{29}$$

$$\frac{1}{\lambda} = -2Mr^2\left(1+\frac{r}{a}\right) - 4\mathrm{i}Mr^3p + \frac{Mr^3(4ra+3a^2+2r^2)}{3a}p^2 + \mathrm{O}(p^3). \tag{30}$$

In the expansion (29), near $p=0$ (corresponding to the minus sign in equation (28)), the linear term is zero. This is in contrast to the expansion for one centre (see equations (14) and (43)) which can be recovered by *first* taking the limit $a\to+\infty$ in the two equations (28) and *then* making a series expansion:

$$\lim_{a\to+\infty} 1/\lambda = -2\frac{Mr\sin(pr)\exp(\mathrm{i}pr)}{p}$$
$$= -2Mr^2 - 2\mathrm{i}Mr^3p + \tfrac{4}{3}Mr^4p^2 + \tfrac{2}{3}\mathrm{i}Mr^5p^3 + \mathrm{O}(p^4).$$

With the definitions

$$\lambda_\mp \equiv -\frac{1}{2Mr^2(1\mp r/a)}$$

the series (29) can be reversed and yields for the poles a fractional power series in the variable $x \equiv 1/\lambda - 1/\lambda_-$:

$$p = \left(\frac{3a}{Mr^3(-3a^2-2r^2+4ar)}\right)^{1/2} x^{1/2} + \mathrm{i}\frac{3a^4}{2Mr^3(-3a^2-2r^2+4ar)^2}x + \mathrm{O}(x^{3/2})$$

and the reversion of the series (30) yields a power series in the variable $y \equiv 1/\lambda - 1/\lambda_+$:

$$p = \mathrm{i}\frac{1}{4Mr^3}\left\{y + \frac{3a^2+2r^2+4ar}{48Mr^3a}y^2 + \mathrm{O}(y^3)\right\}.$$

One deduces from equations (29) and (30) that two bound states exist for $\lambda\langle\lambda_-$, one bound state exists for $\lambda_-\langle\lambda\langle\lambda_+$, and no bound states exist for $\lambda\rangle\lambda_+$. The generalization to a periodic linear chain with more centres (see e.g. [6]) allows the description of a chain with many close energy levels separated by gaps: different spectral regions of high densities of states can be obtained by choosing different suitable λ^ℓ values in the interaction.

4.3. Scattering off a linear chain

The interaction is invariant by rotation about the axis of the chain which will be chosen as the z axis, i.e. the axis of quantization. As a result, the scattering amplitude can be expanded as

$$f(\boldsymbol{p}' \leftarrow \boldsymbol{p}) = \sum_m f_m(\boldsymbol{p}' \leftarrow \boldsymbol{p})$$

and each partial scattering amplitude $f_m(\boldsymbol{p}' \leftarrow \boldsymbol{p})$ can be computed independently. If each interaction V_j is invariant under time reversal, then $f_m = f_{-m}$ and one has

$$f(\boldsymbol{p}' \leftarrow \boldsymbol{p}) = f_0(\boldsymbol{p}' \leftarrow \boldsymbol{p}) + 2\sum_{m\geqslant 1} f_m(\boldsymbol{p}' \leftarrow \boldsymbol{p}).$$

The results simplify further if the initial momentum is parallel to the axis of the chain. Equation (37) then shows that only the $m = 0$ partial amplitude contributes due to the Kronecker symbol in the equation $Y_\ell^m(0, \varphi) = \sqrt{(2\ell + 1)/(4\pi)}\delta_{m0}$, giving

$$f(\boldsymbol{p}' \leftarrow \boldsymbol{p}_\parallel) = f_0(\boldsymbol{p}' \leftarrow \boldsymbol{p}).$$

A numerical application is presented for the three interactions V^0, V^1 , V^2:

$$V^n = \sum_{k=0}^{2} \exp(-\mathrm{i}k\boldsymbol{a}\cdot\boldsymbol{p})v^n \exp(-\mathrm{i}k\boldsymbol{a}\cdot\boldsymbol{p}) \tag{31}$$

$$v^n = \lambda r^3 \sum_{\ell=0}^{n}\sum_{m=-\ell}^{\ell} |r, \ell, m\rangle\langle r, \ell, m|. \tag{32}$$

Each V^n thus represents a linear chain of three identical interactions v^n separated by a distance a. The interaction v^n is effective on the first $n+1$ partial waves with respect to its centre. The range and strength of the interaction are $r = 1$, $\lambda = 100$, and the intercentre separation is $a = 5$.

Figure 2 represents the total cross sections for *one centre only*, versus the momentum $0\langle p\langle 3$ for a particle of unit mass. The curve with circle symbols is for v^0, the curve with

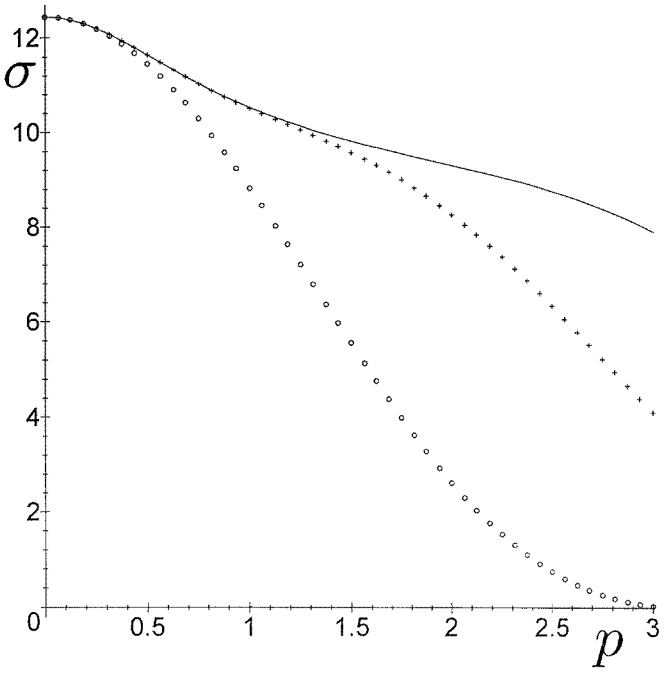

Figure 2. Total cross section σ for scattering by one centre. The abscissa corresponds to the momentum p of the incident particle. The three curves correspond to the three interactions given by equation (32). See text.

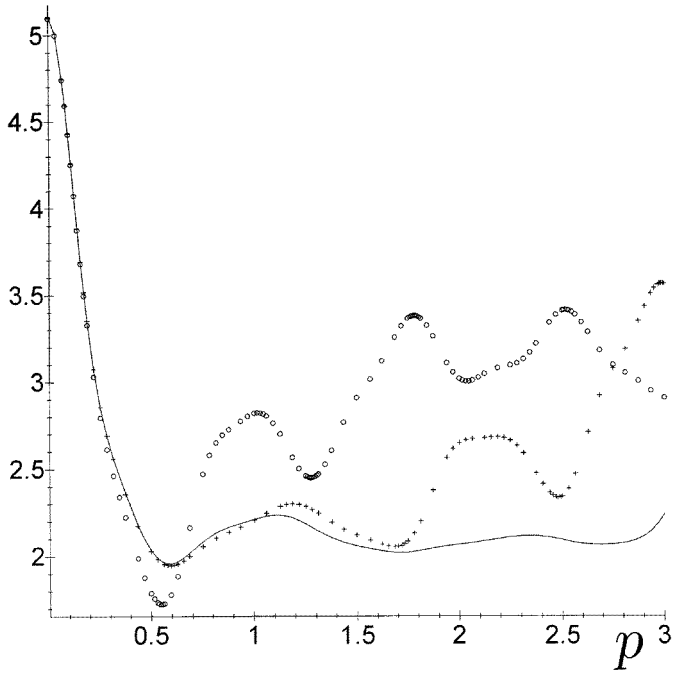

Figure 3. Ratio of the total cross section for scattering off a linear chain of three centres to the total cross section for scattering off one centre only, as a function of the momentum p of the incident particle, parallel to the axis of the chain. For the interactions, see equations (31) and (32).

cross symbols is for v^1, the full curve is for v^2. Figure 3 represents the ratio of the total cross section for the interaction V^n (the linear chain with three centres) to the total cross section for the interaction v^n (one centre only), in the case where the initial momentum is parallel to the axis of the chain. Figure 4 represents the same ratios but for an initial momentum perpendicular to the axis of the chain. The curves with circles, crosses, and the full curve in figures 3 and 4 again correspond to the cases $\ell = 0$, $\ell = \{0, 1\}$, $\ell = \{0, 1, 2\}$ respectively. It is seen that the total cross section is more sensitive to the detail of the interaction and to the energy of the collision for an incident momentum parallel to the chain axis.

A strong anisotropy for scattering by a linear chain is expected [7] at sufficiently high energy due to interference effects. As in optics, one expects the differential cross section to present maxima at well defined scattering angles. Let ω_i, ω_f denote the angles between the initial momentum and the axis of the chain, and the final momentum and the axis of the chain. The maxima for the scattering angle $\theta = \omega_f - \omega_i$ are expected to be given by:

$$\sin(\theta/2) = \frac{n\pi}{pa\sin((\omega_i + \omega_f)/2)} \tag{33}$$

with n integer. For an initial momentum parallel to the axis of the chain ($\omega_i = 0$), equation (33) gives:

$$\theta = 2\arcsin\left(\sqrt{\frac{n\pi}{pa}}\right). \tag{34}$$

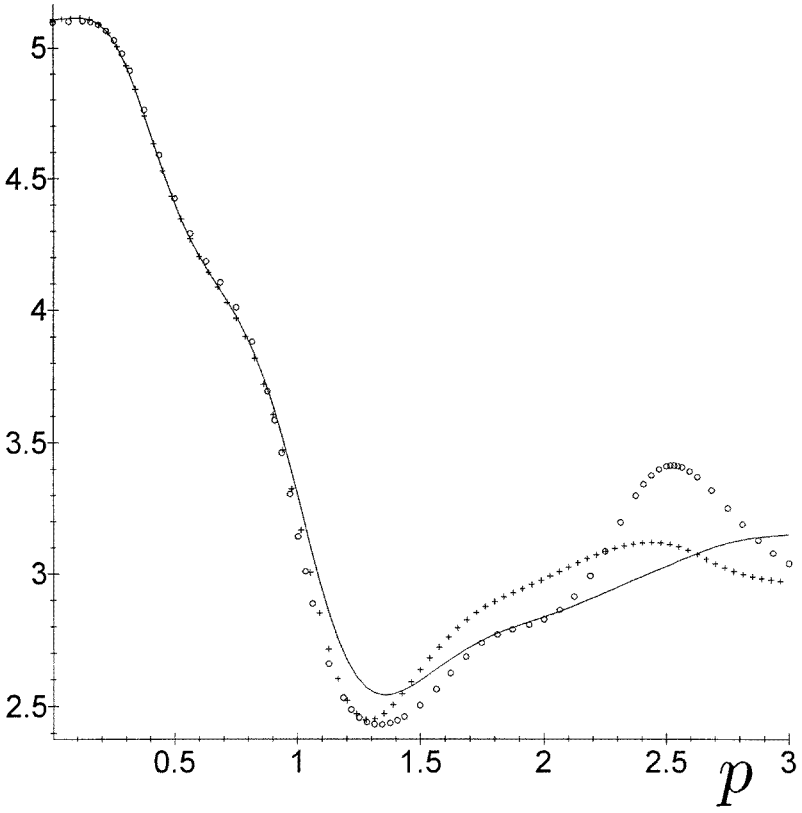

Figure 4. Same as figure 3 but for an initial momentum p perpendicular to the axis of the chain.

This effect is clearly manifested for a chain with only five centres as will now be illustrated. Figure 5 reports the differential cross section *for one centre*, ($r^\ell = 1, \lambda^\ell = 100$ as previously) as a function of the scattering angle θ, for an initial momentum $p = 2$ and a particle of unit mass. The horizontal broken line corresponds to the case where the interaction involves only the s-wave ($\ell = 0$), and the full curve corresponds to the case where the three partial waves $\ell = 0$, $\ell = 1$, $\ell = 2$ are included in the interaction. Figure 6 reports this differential cross section at the same energy, for a chain of five centres, with the intercentre separation $a = 5$, for the case where the initial momentum is parallel to the axis of the chain. In that case, the problem is still invariant under rotation about the axis of the chain and the differential cross section depends only on the angle θ. The curve with circles is for the case where the interaction on each centre involves only the s partial wave $\ell = 0$, the full curve is for the case where the interaction on each centre involves the three partial waves $\ell = \{0, 1, 2\}$. The three angles given by equation (34) for $n = \{1, 2, 3\}$ are reported with symbol V in figure 6. They indeed correspond to three pronounced local maxima of the two curves. The case $n = 0$ of course corresponds to the maximum in the forward direction ($\theta = 0$). The forward scattering peak is much larger than the others for the case where the nonzero partial waves are included in the interaction, whereas its magnitude is equal to the others for the case where only the $\ell = 0$ partial wave is included in the interaction. This is clearly explained by the different behaviour of the differential cross section for one centre presented in figure 5.

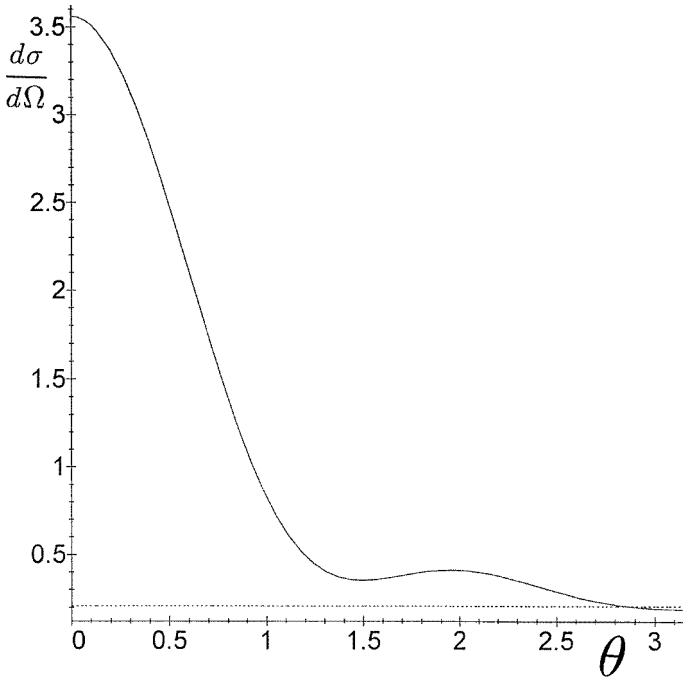

Figure 5. Differential cross section $\mathrm{d}\sigma/\mathrm{d}\Omega$ for scattering off one centre versus the scattering angle θ in radians, for an initial momentum $p = 2$. The full curve correponds to the case where three partial waves are taken into account, the broken line to the case where only the s-wave is taken into account. See text for the details of the interactions.

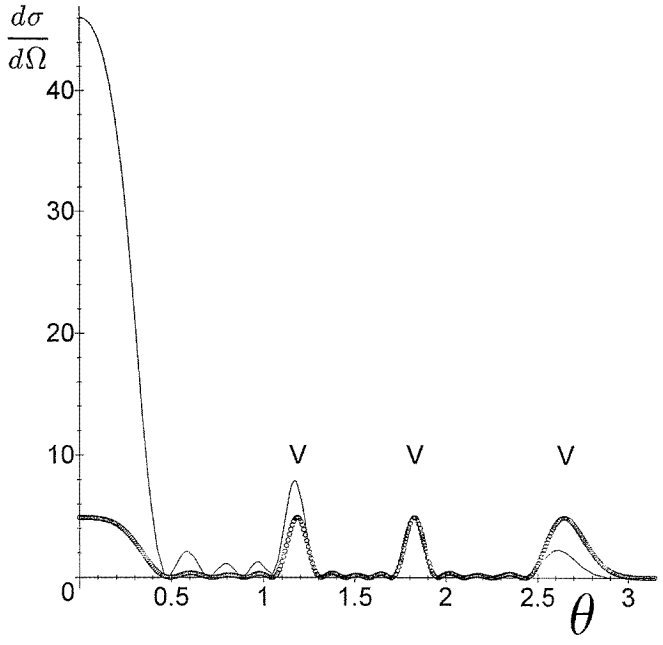

Figure 6. Differential cross section $\mathrm{d}\sigma/\mathrm{d}\Omega$ for scattering off a linear chain of five centres for an initial momentum $p = 2$ parallel to the chain axis, versus the scattering angle in radians. See text.

Acknowledgment

The author would like to thank P Tuckey for helpful discussions and for carefully reading the manuscript.

Appendix A. Normalization and phase conventions

$$
\begin{aligned}
&(L_x \pm \mathrm{i}L_y)|r,\ell,m\rangle = \sqrt{(\ell \pm m + 1)(\ell \mp m)}|r,\ell,m \pm 1\rangle \\
&\langle r',\ell',m'|r,\ell,m\rangle = \frac{\delta(r'-r)}{r^2}\delta_{\ell\ell'}\delta_{mm'} \\
&\langle \boldsymbol{r}'|r,\ell,m\rangle = \frac{\delta(r'-r)}{r^2}Y_\ell^m(\boldsymbol{r}').
\end{aligned}
\tag{35}
$$

(We use for convenience the notation $Y_\ell^m(\boldsymbol{x})$ in place of the more correct notation $Y_\ell^m(\frac{\boldsymbol{x}}{|\boldsymbol{x}|})$.) The spherical harmonic functions Y_ℓ^m are defined as in [8].

$$
\begin{aligned}
1 &= \int \mathrm{d}^3 r|\boldsymbol{r}\rangle\langle\boldsymbol{r}| \\
&= \int_0^\infty \mathrm{d}r\, r^2 \sum_{l=0}^{\infty}\sum_{m=-\ell}^{\ell}|r,\ell,m\rangle\langle r,\ell,m| \\
|r,\ell,m\rangle &= \int \mathrm{d}^3 r' \frac{\delta(r'-r)}{r^2}Y_l^m(\boldsymbol{r}')|\boldsymbol{r}'\rangle \\
&= \int \mathrm{d}\boldsymbol{r}\, Y_l^m(\boldsymbol{r})|\boldsymbol{r}\rangle \\
|\boldsymbol{r}\rangle &= \sum_{l=0}^{\infty}\sum_{m=-\ell}^{\ell}\overline{Y_l^m(\boldsymbol{r})}|r,\ell,m\rangle.
\end{aligned}
\tag{36}
$$

All the above equations remain valid if the letter r is replaced by p with the corresponding interpretation in momentum space. (For example $|\boldsymbol{p}\rangle$ represents a plane wave.)

The relations between these vectors are

$$
\begin{aligned}
&\langle r,\ell,m|p,\ell',m'\rangle = \delta_{\ell\ell'}\delta_{mm'}\mathrm{i}^\ell\sqrt{\frac{2}{\pi}}\,j_\ell(pr) \\
&\langle \boldsymbol{r}|p,\ell,m\rangle = \mathrm{i}^\ell\sqrt{\frac{2}{\pi}}\,j_\ell(pr)Y_\ell^m(\boldsymbol{r}) \\
&\langle \boldsymbol{p}|r,\ell,m\rangle = (-\mathrm{i})^\ell\sqrt{\frac{2}{\pi}}\,j_\ell(pr)Y_\ell^m(\boldsymbol{p}) \\
&(2\pi)^{3/2}\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \exp(\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{p}) = 4\pi\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\mathrm{i}^\ell j_\ell(pr)\overline{Y_\ell^m(\boldsymbol{p})}Y_\ell^m(\boldsymbol{r}).
\end{aligned}
\tag{37}
$$

The spherical Bessel function j_ℓ is related to the usual Bessel function $J_{\ell+\frac{1}{2}}$ which is regular at the origin (see e.g. [9]) by the equation

$$
\begin{aligned}
j_\ell(z) &\equiv \left(\frac{\pi}{2z}\right)^{1/2}J_{\ell+1/2}(z) \\
&= z^\ell\left(-\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^\ell\left(\frac{\sin(z)}{z}\right) \\
&= \frac{\sin(z-\ell\pi/2)}{z}[1+\mathrm{O}(z^{-1})] \qquad \text{as } z\to\infty.
\end{aligned}
\tag{38}
$$

For future convenience the spherical Bessel functions $h_\ell^\pm(z)$ are also now introduced (see e.g. [10]):

$$\begin{aligned} h_\ell^\pm(z) &\equiv (-1)^\ell \left(\frac{\pi}{2z}\right)^{1/2} J_{-\ell-\frac{1}{2}}(z) \pm \mathrm{i} j_\ell(z) \\ &= z^\ell \left(-\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^\ell \left(\frac{\exp(\pm \mathrm{i}z)}{z}\right) \\ &= \frac{\exp(\pm \mathrm{i}(z-\ell\pi/2))}{z}[1+\mathrm{O}(z^{-1})] \qquad \text{as } z \to \infty. \end{aligned} \tag{39}$$

These functions satisfy the following relations which will be used in appendix B:

$$j_\ell(-z) = (-1)^\ell j_\ell(z) \tag{40}$$

$$h_\ell^\pm(-z) = (-1)^{\ell+1} h_\ell^\mp(z). \tag{41}$$

Appendix B. Analytical expressions for matrix elements

B.1. Matrix elements for vectors centred on the same point

The computation of $V_j G_0(z) V_j$ requires the determination of the matrix elements

$$\begin{aligned} \langle \xi_j^k | G_0(z) | \xi_j^q \rangle &= (r_j^k r_j^q)^{3/2} \langle r_j^k, \ell_j^k, m_j^k | G_0(z) | r_j^q, \ell_j^q, m_j^q \rangle \\ &= -\delta_{\ell_j^k \ell_j^q} \delta_{m_j^k m_j^q} 2M (r_j^k r_j^q)^{3/2} p h_{\ell_j^k}^+(pr_\rangle) j_{\ell_j^k}(pr_\langle) \end{aligned} \tag{42}$$

where $r_\rangle$, $r_\langle$ denote respectively the greatest and lowest value of r_j^k, r_j^q, (equal in the case $r_j^k = r_j^q$), and p is given by equation (10).

The Kronecker symbols in equation (42) express the fact that $G_0(z)$ commutes with the angular momentum operators, and the derivation of equation (42) requires an integration in the complex p plane and is given for example in [2]. For the particular case $\ell_j^k = m_j^k = 0$, $r_j^k \equiv r$, equation (42) gives:

$$r^3 \langle r, 0, 0 | G_0(z) | r, 0, 0 \rangle = -2Mr^3 p \left(\frac{\exp(\mathrm{i}pr)}{pr}\right)\left(\frac{\sin(pr)}{pr}\right). \tag{43}$$

B.2. Matrix elements for vectors centred on different points

The computation of $V_j G_0(z) V_s$ $(j \neq s)$ requires the determination of the matrix elements

$$\begin{aligned} \langle \xi_j^k | G_0(z) | \xi_s^q \rangle &= (r_j^k r_s^q)^{3/2} \langle r_j^k, \ell_j^k, m_j^k | \exp(\mathrm{i}\boldsymbol{a}_j \cdot \boldsymbol{p}) G_0(z) \exp(-\mathrm{i}\boldsymbol{a}_s \cdot \boldsymbol{p}) | r_s^q, \ell_s^q, m_s^q \rangle \\ &= (r_j^k r_s^q)^{3/2} \langle r_j^k, \ell_j^k, m_j^k | \exp(-\mathrm{i}(\boldsymbol{a}_s - \boldsymbol{a}_j) \cdot \boldsymbol{p}) G_0(z) | r_s^q, \ell_s^q, m_s^q \rangle. \end{aligned}$$

An expansion of the exponential term according to equation (37) and the insertion of the closure relation (36) with p in place of r yields

$$\begin{aligned} \langle \xi_j^k | G_0(z) | \xi_s^q \rangle &= (r_j^k r_s^q)^{3/2} 8 \sum_{\lambda,\mu} \mathrm{i}^{(\lambda+\ell_j^k-\ell_s^q)} \overline{Y_\lambda^\mu(\boldsymbol{a}_j - \boldsymbol{a}_s)} \\ &\quad \times \int_0^\infty \mathrm{d}p\, p^2 \frac{j_{\ell_j^k}(pr_j^k) j_{\ell_s^q}(pr_s^q) j_\lambda(p|\boldsymbol{a}_j - \boldsymbol{a}_s|)}{z - p^2/(2M)} \int \mathrm{d}\hat{p}\, \overline{Y_{\ell_j^k}^{m_j^k}(\boldsymbol{p})} Y_{\ell_s^q}^{m_s^q}(\boldsymbol{p}) Y_\lambda^\mu(\boldsymbol{p}). \end{aligned}$$

The angular integration over the product of three spherical harmonics can be expressed in terms of Wigner $3j$ symbols (see e.g. [8]):

$$\int \mathrm{d}\hat{p} \overline{Y_{\ell_j^k}^{m_j^k}(p)} Y_{\ell_s^q}^{m_s^q}(p) Y_\lambda^\mu(p)$$

$$= (-1)^{-m_j^k}\sqrt{\frac{(2\ell_j^k+1)(2\ell_s^q+1)(2\lambda+1)}{4\pi}}\begin{pmatrix} l_j^k & l_s^q & \lambda \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_j^k & l_s^q & \lambda \\ -m_j^k & m_s^q & \mu\end{pmatrix}.$$

It is important to note that the $3j$ symbols with only zeros on the second line are different from zero only if $l_j^k + l_s^q + \lambda$ is even. The computation of the radial integral

$$B \equiv \int_0^\infty \mathrm{d}p\, p^2 \frac{j_{\ell_j^k}(pr_j^k) j_{\ell_s^q}(pr_s^q) j_\lambda(p|\boldsymbol{a}_j - \boldsymbol{a}_s|)}{z - p^2/(2M)}$$

then goes as follows. From equation (40) and the even parity of the sum $l_j^k + l_s^q + \lambda$, one deduces

$$B = \frac{1}{2}\int_{-\infty}^\infty \mathrm{d}p\, p^2 \frac{j_{\ell_j^k}(pr_j^k) j_{\ell_s^q}(pr_s^q) j_\lambda(p|\boldsymbol{a}_j - \boldsymbol{a}_s|)}{z - p^2/(2M)}.$$

The decomposition

$$j_\lambda(p|\boldsymbol{a}_j - \boldsymbol{a}_s|) = \frac{h_\lambda^+(p|\boldsymbol{a}_j - \boldsymbol{a}_s|) - h_\lambda^-(p|\boldsymbol{a}_j - \boldsymbol{a}_s|)}{2\mathrm{i}}$$

and the inequalities

$$|\boldsymbol{a}_j - \boldsymbol{a}_s| \geqslant r_s^q + r_j^k \tag{44}$$

allow the closure of the contour with an infinite semi circle in the upper half plane for the part involving h^+ and with an infinite semi circle in the lower half plane for the part involving h^-, without changing the value of B. The Cauchy theorem on residues then yields

$$B = \frac{M}{2\mathrm{i}} 2\pi\mathrm{i}\frac{p}{2}\{-j_{\ell_j^k}(pr_j^k) j_{\ell_s^q}(pr_s^q) h_\lambda^+(p|\boldsymbol{a}_j - \boldsymbol{a}_s|) + j_{\ell_j^k}(-pr_j^k) j_{\ell_s^q}(-pr_s^q) h_\lambda^-(-p|\boldsymbol{a}_j - \boldsymbol{a}_s|)\}$$

with p given by equation (10). From equations (40) and (41), one finally obtains

$$\begin{aligned}\langle \xi_j^k | G_0(z) | \xi_s^q \rangle &= -(-1)^{m_j^k}(r_j^k r_s^q)^{3/2} 8\pi M p j_{\ell_j^k}(pr_j^k) j_{\ell_s^q}(pr_s^q)\sqrt{\frac{(2\ell_j^k+1)(2\ell_s^q+1)}{4\pi}} \\ &\times \sum_\lambda \sqrt{2\lambda+1}\,\mathrm{i}^{(\lambda+\ell_j^k-\ell_s^q)} h_\lambda^+(p|\boldsymbol{a}_j - \boldsymbol{a}_s|)\overline{Y_\lambda^{m_j^k - m_s^q}(\boldsymbol{a}_j - \boldsymbol{a}_s)} \\ &\begin{pmatrix} l_j^k & l_s^q & \lambda \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_j^k & l_s^q & \lambda \\ -m_j^k & m_s^q & m_j^k - m_s^q\end{pmatrix}.\end{aligned} \tag{45}$$

The λ values which contribute to the above sum are those which satisfy $|\ell_j^k - \ell_s^q| \langle \lambda \langle \ell_j^k + \ell_s^q$ and $\lambda + \ell_j^k + \ell_s^q$ even. For the particular case $\ell_j^k = \ell_s^q = m_j^k = m_s^q = 0, r_j^k = r_s^q \equiv r$, equation (45) gives:

$$\begin{aligned}&r^3\langle r,0,0|\exp(\mathrm{i}\boldsymbol{a}_j\cdot\boldsymbol{p})G_0(z)\exp(-\mathrm{i}\boldsymbol{a}_s\cdot\boldsymbol{p})|r,0,0\rangle \\ &\qquad = -2Mr^3 p\left(\frac{\sin(pr)}{pr}\right)^2\left(\frac{\exp(\mathrm{i}p|\boldsymbol{a}_j - \boldsymbol{a}_s|)}{p|\boldsymbol{a}_j - \boldsymbol{a}_s|}\right).\end{aligned} \tag{46}$$

Appendix C. Symmetry properties with respect to rotation, time reversal and parity

C.1. Invariance properties of each interaction V_j

First let us consider the behaviour of each interaction V_j (see equations (3) and (4)) under rotation *with respect to its centre* P_j (see equation (2)).

$$\exp(-\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{L})|r,l,m\rangle=\sum_{m'}D^{\ell}_{m',m}(\boldsymbol{\alpha})|r,l,m'\rangle$$

where $\boldsymbol{\alpha}$ is the vector which defines the rotation, and $D^{\ell}_{m',m}(\boldsymbol{\alpha})$ are the elements of the rotation matrices which are defined here as in [8] except for the sign of the argument $\boldsymbol{\alpha}$. The unitarity properties of these matrices

$$\sum_{m}D^{\ell}_{m',m}(\boldsymbol{\alpha})\overline{D^{\ell}_{m'',m}(\boldsymbol{\alpha})}=\delta_{m',m''}$$

imply that rotational invariance of V_j requires that V_j must involve the whole sum $\sum_{m=-\ell}^{\ell}|r,\ell,m\rangle\langle r,\ell,m|$ for each value of r,ℓ considered.

If T denotes the time-reversal operator, the equation

$$T|r,\ell,m\rangle=(-1)^m|r,\ell,-m\rangle$$

implies that time-reversal invariance requires that V_j must involves the sum $|r,\ell,m\rangle\langle r,\ell,m|+|r,\ell,-m\rangle\langle r,\ell,-m|$ for each value of r,ℓ considered. Therefore, if the interaction V_j is invariant under rotation, it is also invariant under time reversal.

The equation

$$P|r,l,m\rangle=(-1)^{\ell}|r,\ell,m\rangle \tag{47}$$

where P is the reflection operator, shows that V_j is always invariant by reflection *with respect to its centre.*

C.2. Symmetry properties of the matrix elements of the free resolvent G_0

The solution of the scattering problem requires the computation of following matrix elements of the operator $B\equiv\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})G_0(z)$ (see equations (42) and (45)):

$$A\equiv\langle r,\ell,m|B|r',\ell',m'\rangle.$$

It is therefore of interest to find the symmetry properties relevant to these matrix elements.

C.2.1. General symmetry properties. By general properties, we mean properties that are independent of the relative orientation of Oz and $\boldsymbol{a}-\boldsymbol{a}'$. The property

$$A=(-1)^{m+m'}\langle r',\ell',-m'|\exp(\mathrm{i}(\boldsymbol{a}'-\boldsymbol{a})\cdot\boldsymbol{p})G_0(z)|r,\ell,-m\rangle$$

can be obtained directly from consideration of time reversal. For the proof, it is convenient to use the scalar product notation $\langle,T\rangle$ in place of the Dirac notation $\langle|T|\rangle$ which can be ambiguous for anti-unitary operators [2]: $\langle\psi,T\chi\rangle=\overline{\langle T^{\dagger}\psi,\chi\rangle}$

$$\begin{aligned}A&=\langle(r,\ell,m),\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})T^{\dagger}TG_0(z)T^{\dagger}T(r',\ell',m')\rangle\\&=\langle(r,\ell,m),\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})T^{\dagger}G_0(\bar{z})T(r',\ell',m')\rangle\\&=(-1)^{m'}\langle(r,\ell,m),T^{\dagger}\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})G_0(\bar{z})(r',\ell',-m')\rangle\\&=(-1)^{m+m'}\langle r',\ell',-m'|\exp(\mathrm{i}(\boldsymbol{a}'-\boldsymbol{a})\cdot\boldsymbol{p})G_0(z)|r,\ell,-m\rangle.\end{aligned}$$

Equation (47) shows that

$$A=(-1)^{\ell+\ell'}\langle r,\ell,m|\exp(-\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})G_0(z)|r',\ell',m'\rangle.$$

C.2.2. Symmetry properties for special geometric configurations The rotation operator $\exp(-\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{L})$ associated with a rotation of angle α around an axis with polar coordinate θ,φ can be expressed in terms of our fixed frame O,x,y,z operators:

$$\exp(-\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{L}) = \exp(-\mathrm{i}\varphi L_z)\exp(-\mathrm{i}\theta L_y)\exp(-\mathrm{i}\alpha L_z)\exp(\mathrm{i}\theta L_y)\exp(\mathrm{i}\varphi L_z). \tag{48}$$

We shall use the definition $\langle \ell, m|\exp(-\mathrm{i}\beta L_y)|l', m'\rangle \equiv d^{\ell}_{mm'}(\beta)$ and with the phase convention (35):

$$d^{\ell}_{mm'}(-\beta) = (-1)^{m'-m} d^{\ell}_{mm'}(\beta)$$
$$d^{\ell}_{mm'}(\pi) = (-1)^{\ell-m'}\delta_{m',-m}.$$

The notation $d^{\ell}_{mm'}(\beta)$ differs from that of [8] by the sign of β. Let us now consider rotations of centre O along an axis parallel to the vector $\boldsymbol{a}-\boldsymbol{a}'$, and of angle α. The unitary rotation operator $\exp(-\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{L})$ associated with this operation clearly commute with B, and the equation $A = \langle r,\ell,m|\exp(\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{L})B\exp(-\mathrm{i}\boldsymbol{\alpha}\cdot\boldsymbol{L})|r',\ell',m'\rangle$ yields according to equation (48):

- $A = 0$ if $m \neq m'$ for the case $\boldsymbol{a}'-\boldsymbol{a}$ parallel to Oz.
- $A = (-1)^{\ell+m+\ell'+m'}\langle r',\ell',-m'|\exp(\mathrm{i}(\boldsymbol{a}'-\boldsymbol{a})\cdot\boldsymbol{p})G_0(z)|r,\ell,-m\rangle$ for the case $\boldsymbol{a}'-\boldsymbol{a}$ parallel to Oy. (This result is obtained by considering a rotation of angle π).
- $A = (-1)^{\ell+\ell'}\langle r',\ell',-m'|\exp(\mathrm{i}(\boldsymbol{a}'-\boldsymbol{a})\cdot\boldsymbol{p})G_0(z)|r,\ell,-m\rangle$ for the case $\boldsymbol{a}'-\boldsymbol{a}$ parallel to Ox. (This result is obtained by considering a rotation of angle π.)

Finally, the unitary operator U associated with reflection with respect to a *plane* containing the vector $\boldsymbol{a}-\boldsymbol{a}'$ clearly commutes with B. U is equal to the parity operator P left multiplied by the rotation operator corresponding to a π rotation about an axis perpendicular to the plane. If $\theta_\perp,\varphi_\perp$ denote the polar and azimuthal angles of a vector perpendicular to the plane, it can be shown by considering equation (48), that the equation $A = \langle r,\ell,m|U^\dagger BU|r',\ell',m'\rangle$ can be expressed as:

$$A = (-1)^{\ell+m+\ell'+m'}\exp(\mathrm{i}(m'-m)\varphi_\perp)\sum_{\mu,\mu'}\exp(\mathrm{i}(\mu-\mu')\varphi_\perp)d^{\ell'}_{\mu'm'}(2\theta_\perp)d^{\ell}_{\mu m}(2\theta_\perp)\langle r,\ell,\mu|$$
$$\times\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})G_0(z)|r',\ell',\mu'\rangle. \tag{49}$$

One deduces from equation (49):

- $A = 0$ if $\ell+m+\ell'+m'$ odd for $\boldsymbol{a}-\boldsymbol{a}'$ in the plane Ox, Oy (by choosing $\theta_\perp = 0$).
- $A = \langle r,\ell,-m|\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})G_0(z)|r',\ell',-m'\rangle$ for $\boldsymbol{a}-\boldsymbol{a}'$ in the plane Oy, Oz (by choosing $\theta_\perp = \pi/2, \varphi_\perp = 0$).
- $A = (-1)^{m'-m}\langle r,\ell,-m|\exp(\mathrm{i}(\boldsymbol{a}-\boldsymbol{a}')\cdot\boldsymbol{p})G_0(z)|r',\ell',-m'\rangle$ for $\boldsymbol{a}-\boldsymbol{a}'$ in the plane Ox, Oz (by choosing $\theta_\perp = \pi/2, \varphi_\perp = \pi/2$).

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